Exascale Challenges for the Applied Mathematics and Computer Science Community

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Key Message

- The transition from petascale to exascale will be characterized by significant and dramatics changes in hardware and architecture.
- This transition will be disruptive, but create unprecedented opportunities for computational science.

Overview

- From 1999 to 2009: evolution from Teraflops to Petaflops computing
- From 2010 to 2020: key technology changes towards Exaflops computing
- Impact on Applied Mathematics

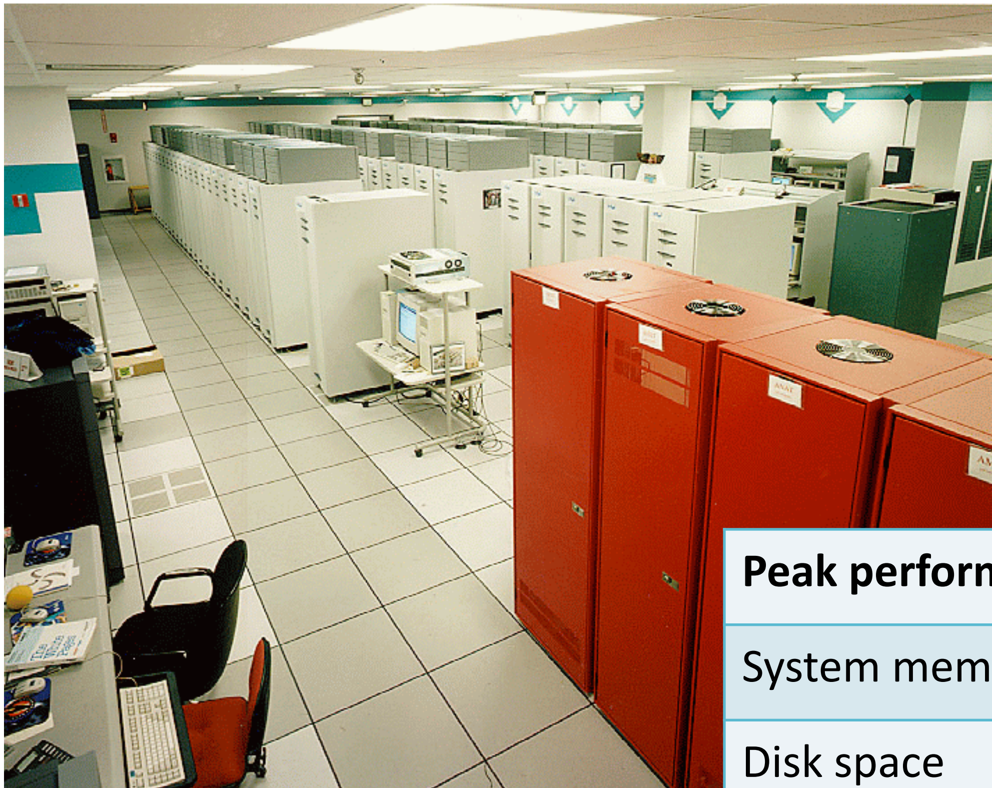
Jaguar: World's most powerful computer in 2009

Peak performance	**2.332 PF**
System memory	300 TB
Disk space	10 PB
Processors	224K
Power	6.95 MW

TOP500® SUPERCOMPUTER SITES

#1 Nov. 2009

ASCI Red: World's Most Powerful Computer in 1999



TOP500 SUPERCOMPUTER SITES

#1 Nov. 1999

Peak performance	**3.154 TF**
System memory	1.212 TB
Disk space	12.5 TB
Processors	9298
Power	850 kW

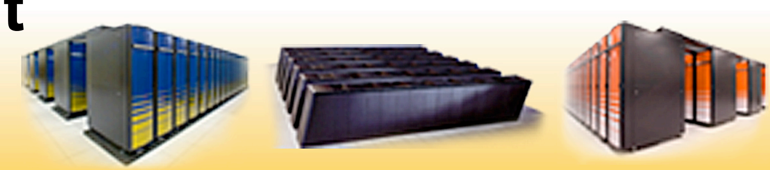
Comparison
Jaguar (2009) vs. ASCI Red (1999)

- **739x performance (LINPACK)**
- **267x memory**
- **800x disk**
- **24x processors/cores**
- **8.2x power**

Parallelism and faster processors made about equal contributions to performance increase

Significant increase in operations cost

Essentially the same architecture and software environment



Overview

- **From 1999 to 2009: evolution from Teraflops to Petaflops computing**
- **From 2010 to 2020: key technology changes towards Exaflops computing**
- **Impact on Applied Mathematics**

Traditional Sources of Performance Improvement are Flat-Lining (2004)

- **New Constraints**
  - 15 years of *exponential* clock rate growth has ended
- **Moore's Law reinterpreted:**
  - How do we use all of those transistors to keep performance increasing at historical rates?
  - Industry Response: #cores per chip doubles every 18 months *instead* of clock frequency!

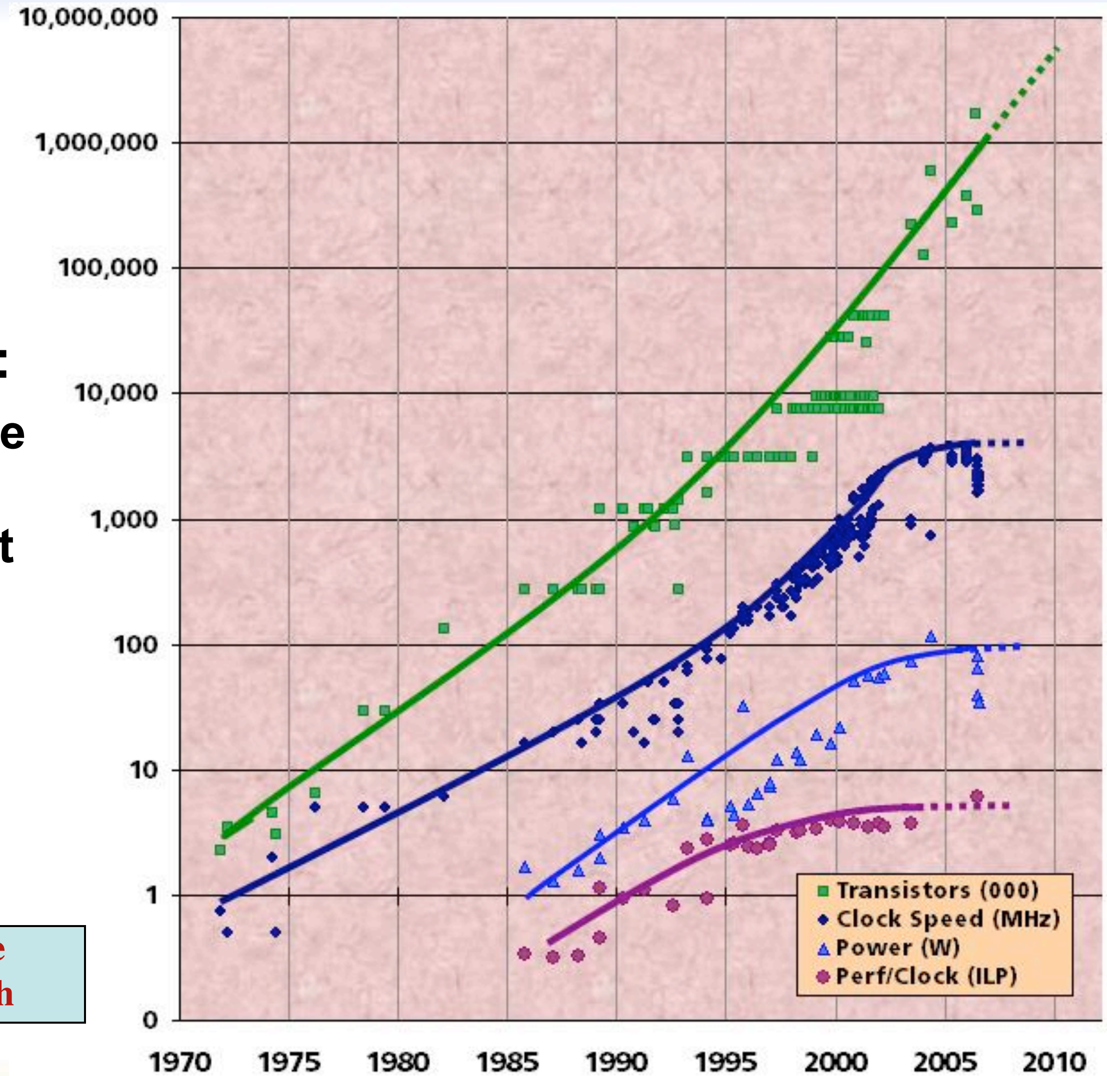
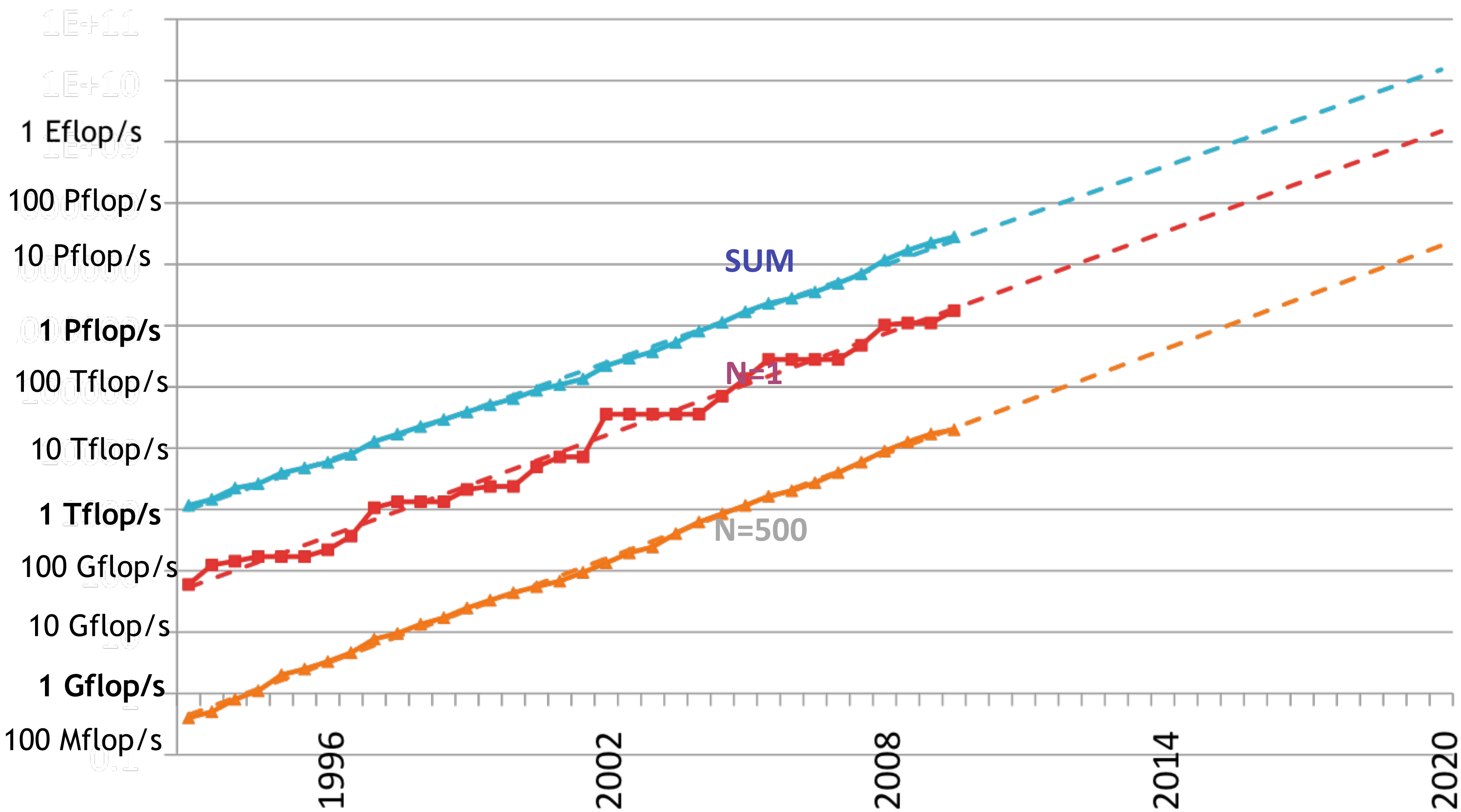
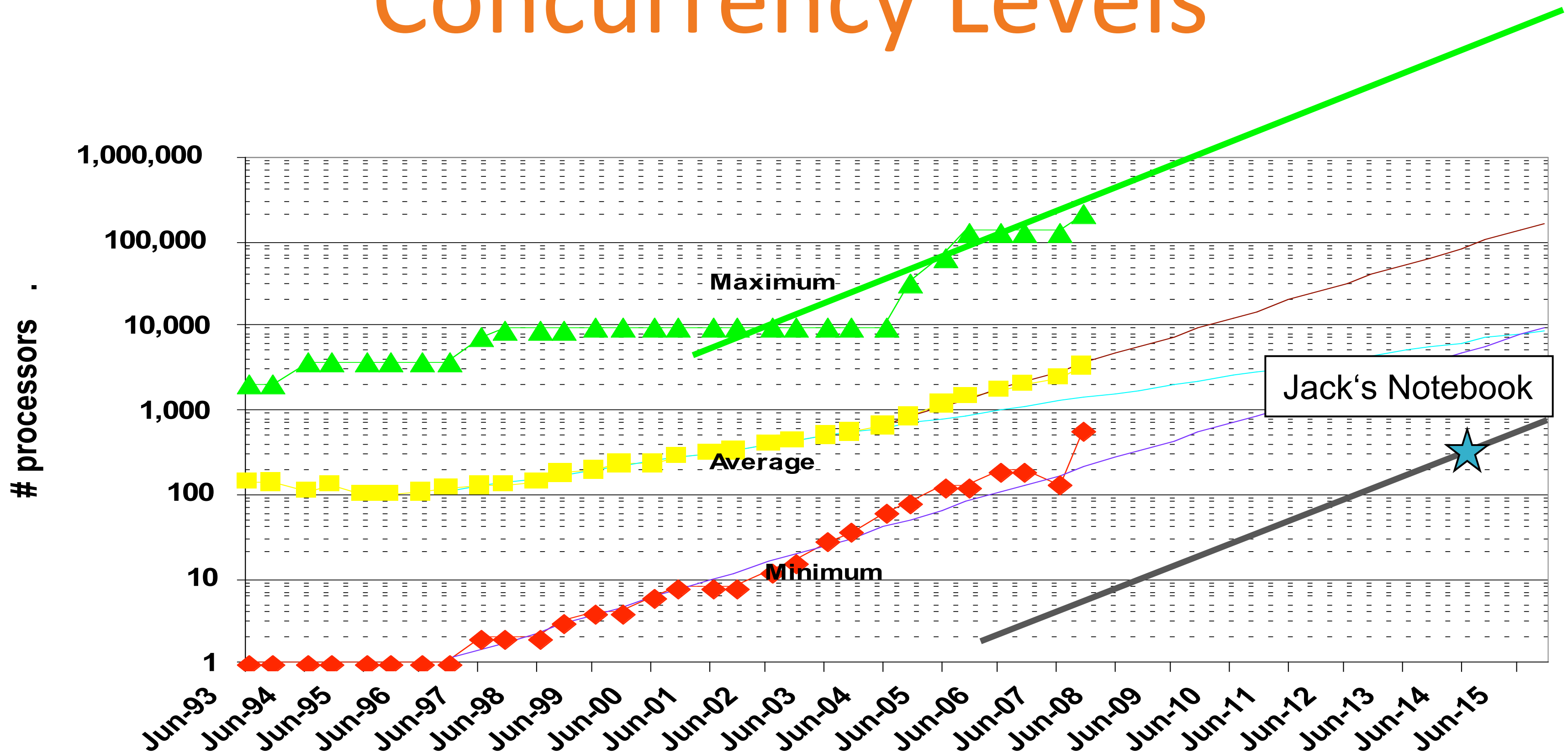


Figure courtesy of Kunle Olukotun, Lance Hammond, Herb Sutter, and Burton Smith

Projected Performance Development

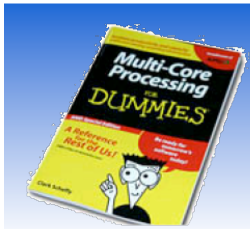


Concurrency Levels



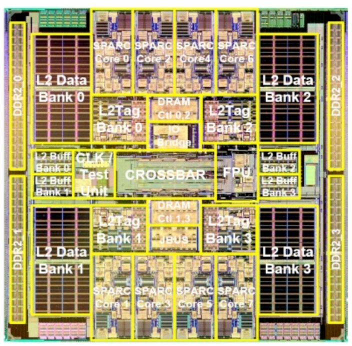
Moore's Law reinterpreted

- Number of cores per chip will double every two years
- Clock speed will not increase (possibly decrease)
- Need to deal with systems with millions of concurrent threads
- Need to deal with inter-chip parallelism as well as intra-chip parallelism

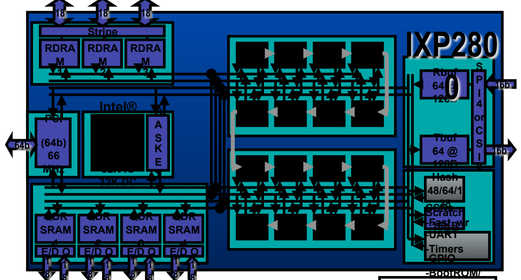


Multicore comes in a wide variety

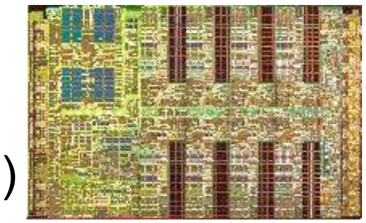
- Multiple parallel general-purpose processors (GPPs)
- Multiple application-specific processors (ASPs)

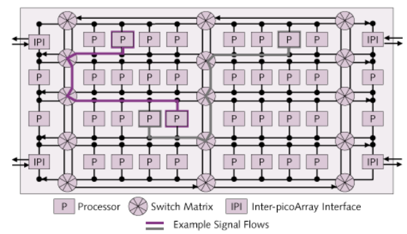


Intel Network Processor
1 GPP Core
16 ASPs (128 threads)



IBM Cell
1 GPP (2 threads)
8 ASPs

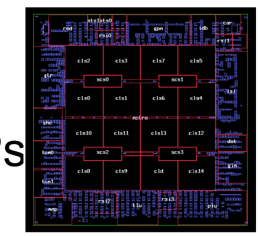


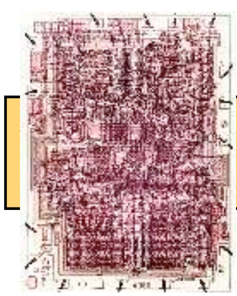


Picochip DSP
1 GPP core
248 ASPs

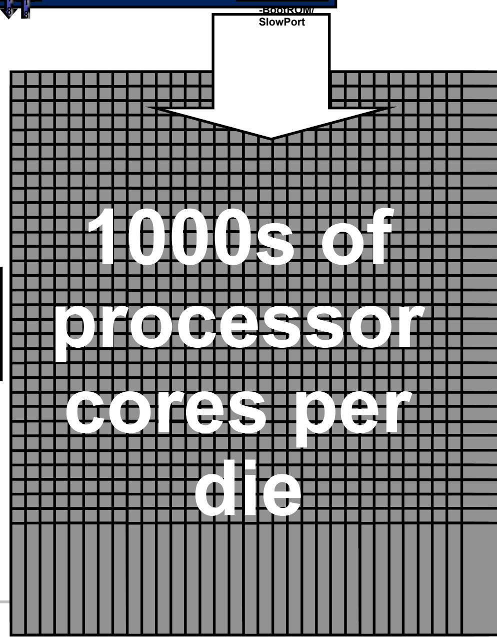
Sun Niagara
8 GPP cores (32 threads)

Cisco CRS-1
188 Tensilica GPPs



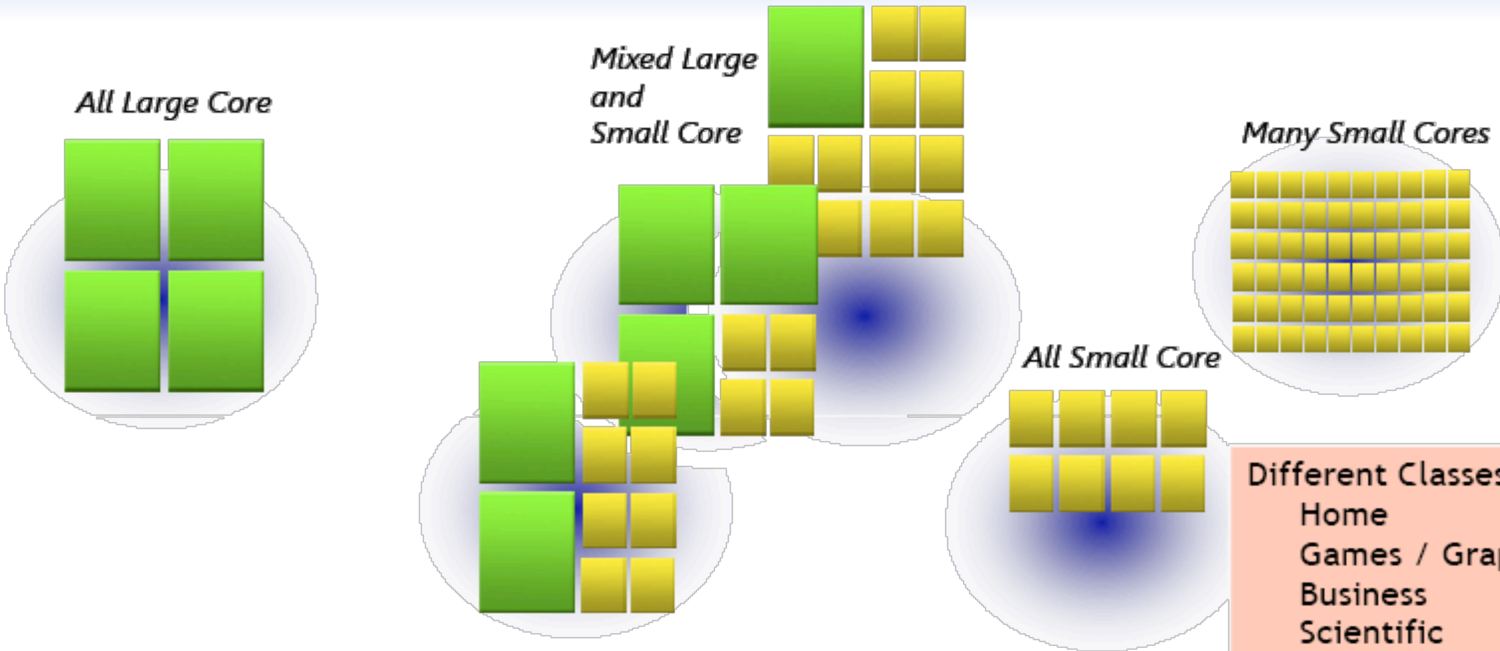


Intel 4004 (1971):
4-bit processor,
2312 transistors,
~100 KIPS,
10 micron PMOS,
11 mm² chip



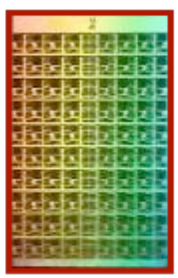
"The Processor is the new Transistor" [Rowen]

What's Next?

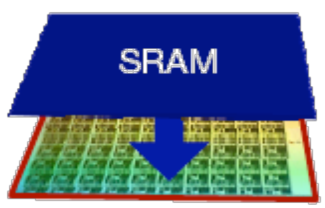


Different Classes of Chips
- Home
- Games / Graphics
- Business
- Scientific

Many Floating-Point Cores



+ 3D Stacked Memory

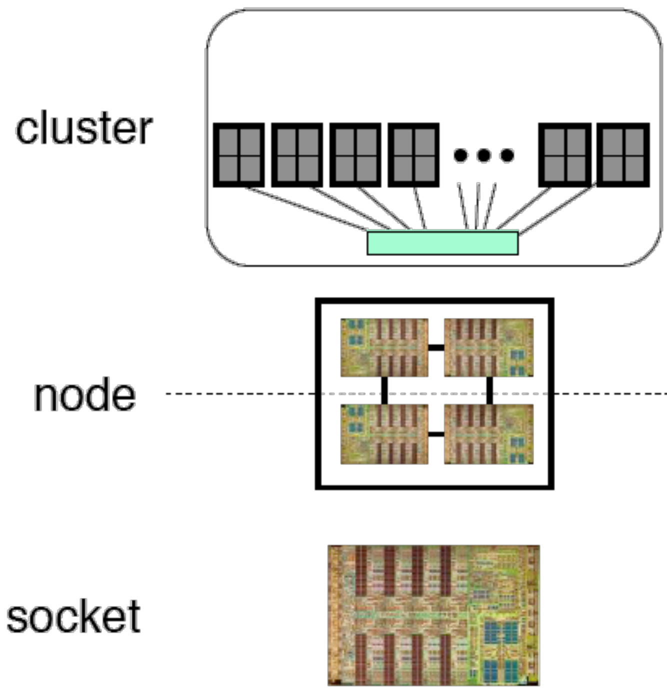


The question is not whether this will happen but whether we are ready

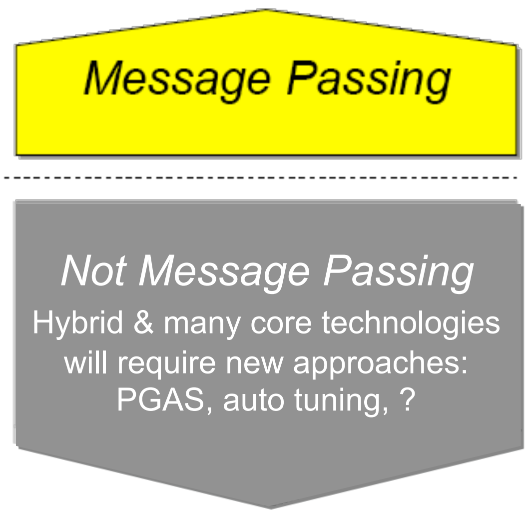
Source: Jack Dongarra, ISC 2008

Roadrunner - A Likely Future Scenario

System: cluster + many core node



Programming model: MPI+X



after Don Grice, IBM, Roadrunner Presentation, ISC 2008

Why MPI will persist

- Obviously MPI will not disappear in five years
- By 2014 there will be 20 years of legacy software in MPI
- New systems are not sufficiently different to lead to new programming model

What will be the “X” in MPI+X

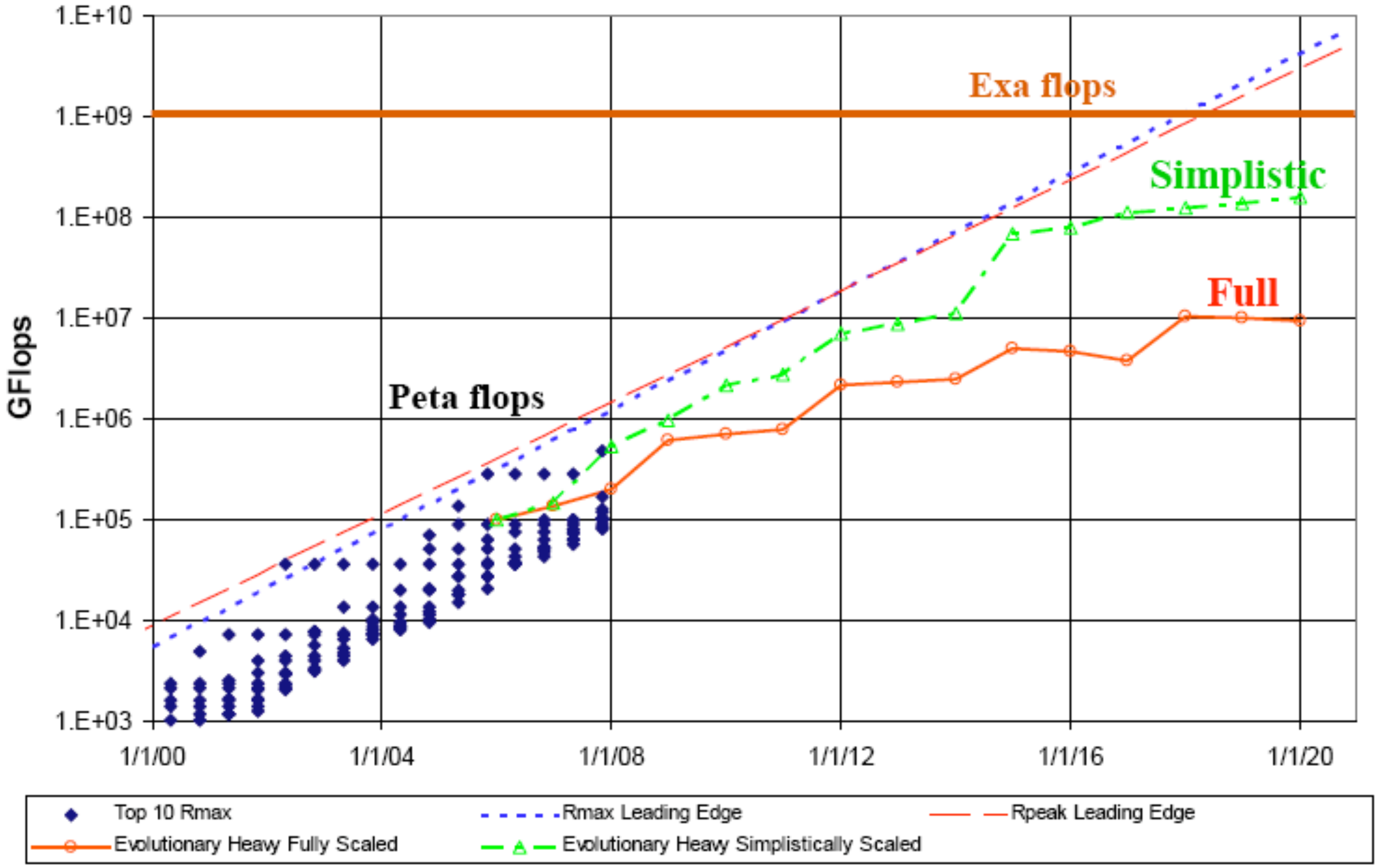
- **Likely candidates are**
  - – PGAS languages
  - – OpenMP
  - – Autotuning
  - – CUDA, OpenCL
  - – A wildcard from commercial space

What’s Wrong with MPI Everywhere?

What's Wrong with MPI Everywhere?

- One MPI process per core is wasteful of intra-chip latency and bandwidth
- Weak scaling: success model for the "cluster era"
  - not enough memory per core
- Heterogeneity: MPI per CUDA thread-block?

We won't reach Exaflops with the current approach



From Peter Kogge, DARPA Exascale Study

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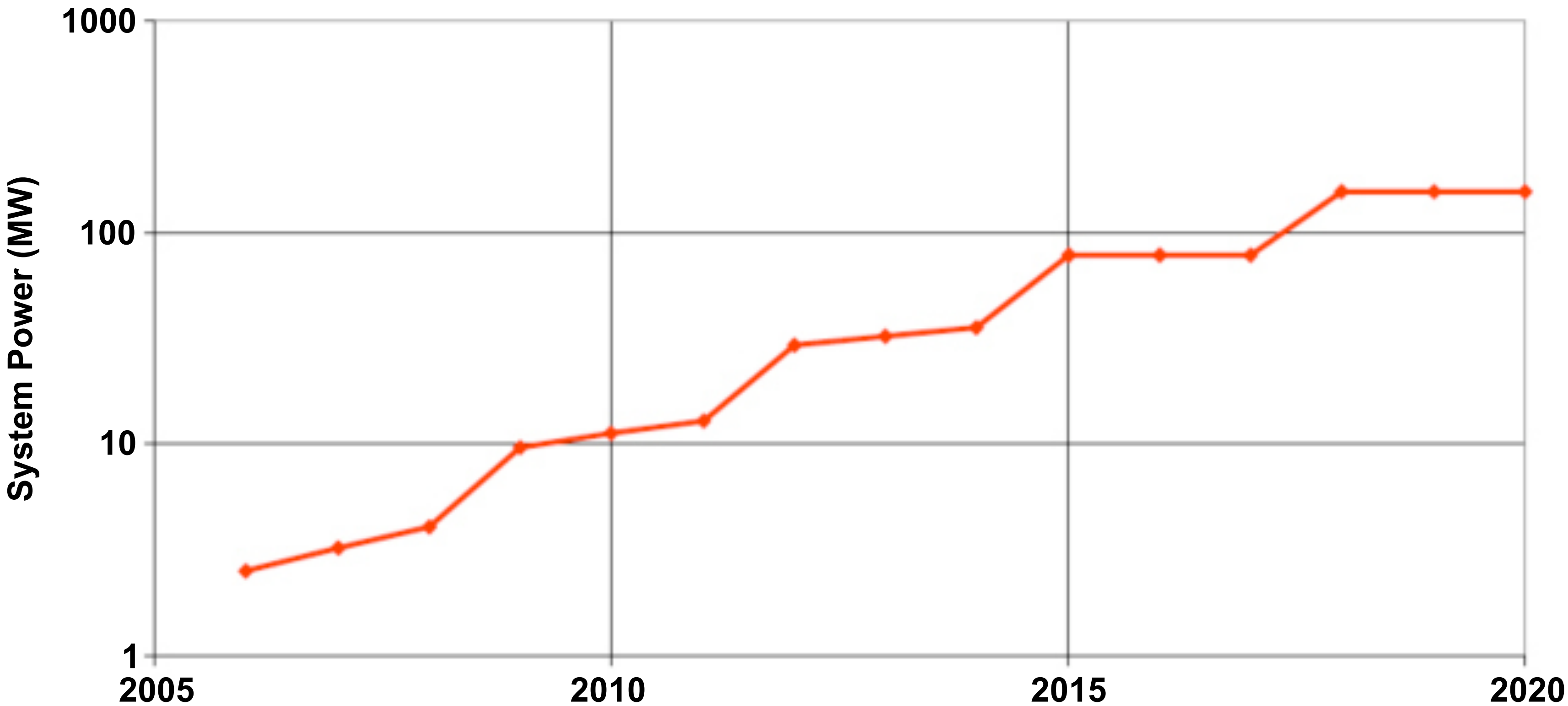
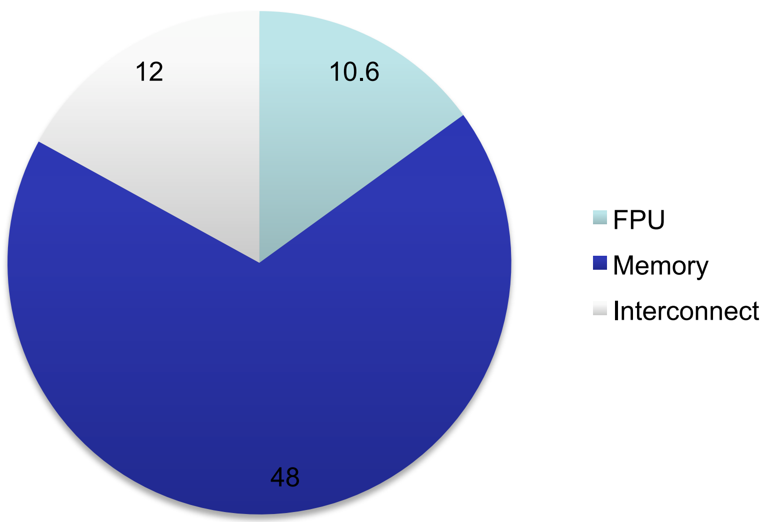
… and the power costs will still be staggering



From Peter Kogge,
DARPA Exascale Study

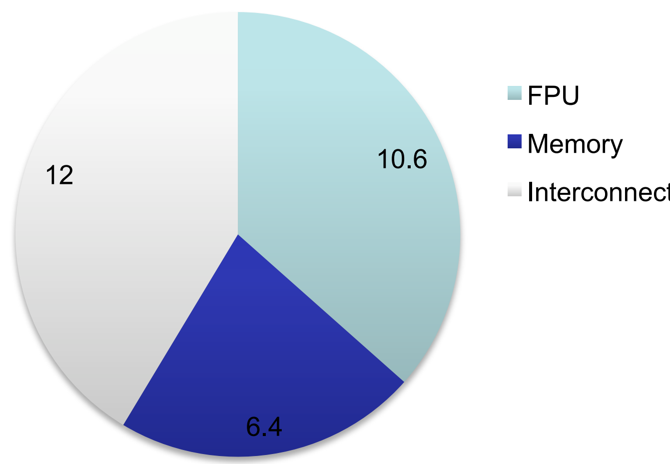
Memory Power Consumption

- Power Consumption with standard Technology Roadmap



70 Megawatts total

- Power Consumption with Investment in Advanced Memory Technology



20 Megawatts total

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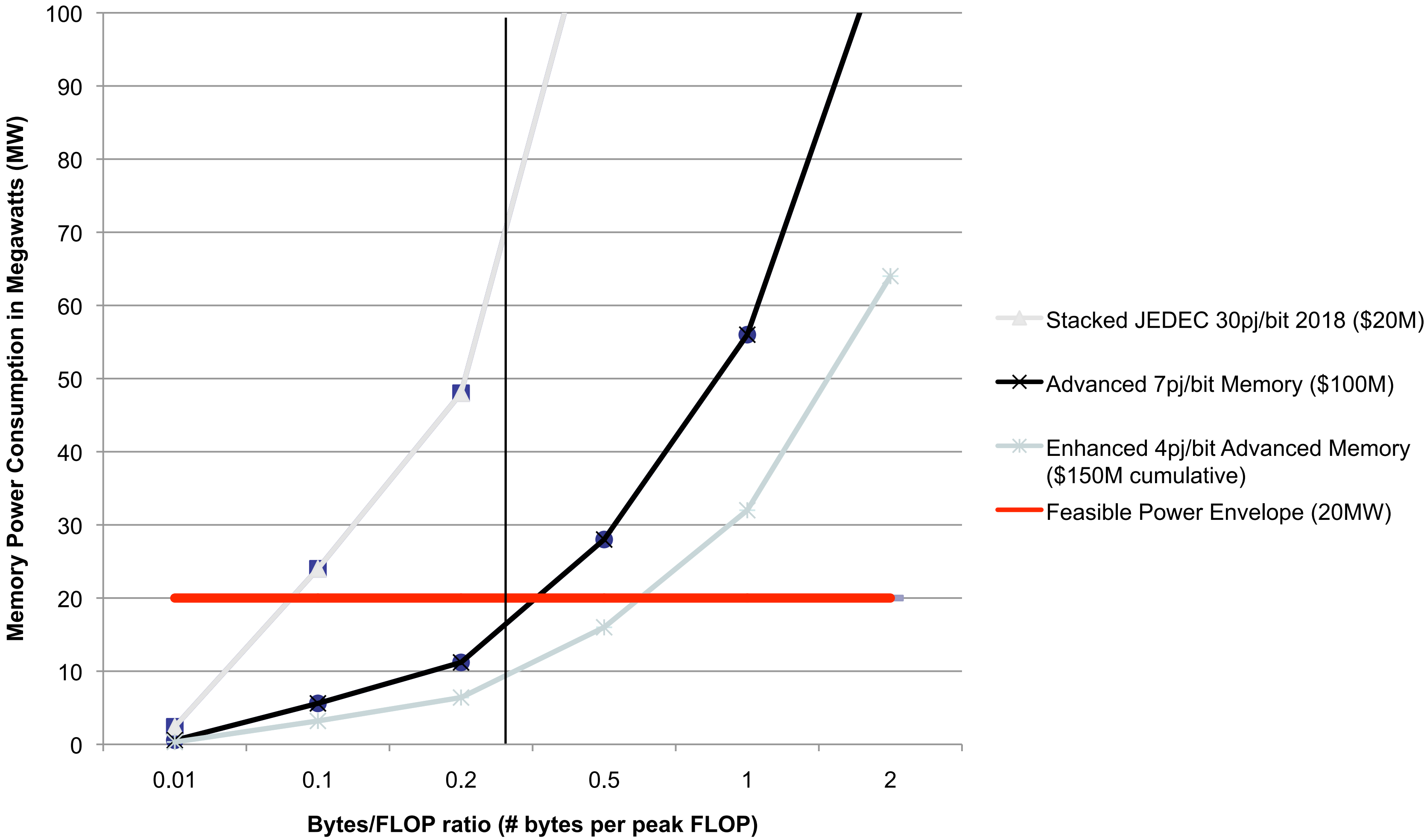
Memory Technology
Bandwidth costs power



A decadal DOE plan for providing exascale applications and technologies for DOE mission needs

Rick Stevens and Andy White, co-chairs

Pete Beckman, Ray Bair-ANL; Jim Hack, Jeff Nichols, Al Geist-ORNL; Horst Simon, Kathy Yelick, John Shalf-LBNL; Steve Ashby, Moe Khaleel-PNNL; Michel McCoy, Mark Seager, Brent Gorda-LLNL; John Morrison, Cheryl Wampler-LANL; James Peery, Sudip Dosanjh, Jim Ang-SNL; Jim Davenport, Tom Schlagel, BNL; Fred Johnson, Paul Messina, ex officio

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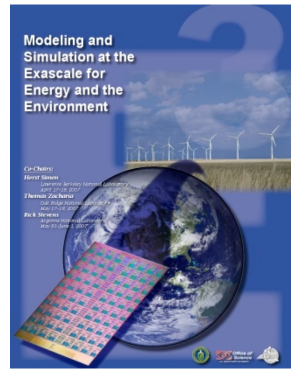
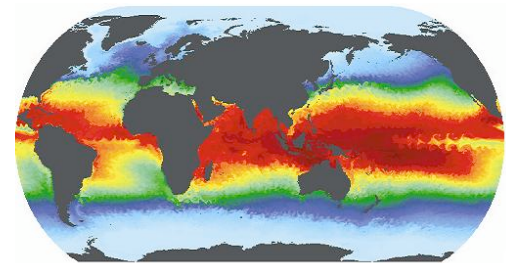
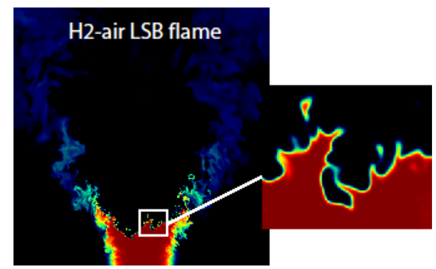
Process for identifying exascale applications and technology for DOE missions ensures broad community input

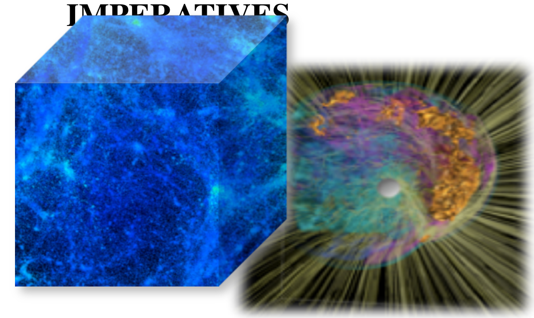
- **Town Hall Meetings April-June 2007**
- **Scientific Grand Challenges Workshops Nov, 2008 – Oct, 2009**
  - **Climate Science (11/08),**
  - **High Energy Physics (12/08),**
  - **Nuclear Physics (1/09),**
  - **Fusion Energy (3/09),**
  - **Nuclear Energy (5/09),**
  - **Biology (8/09),**
  - **Material Science and Chemistry (8/09),**
  - **National Security (10/09)**
  - **Cross-cutting technologies (2/10)**
- **Exascale Steering Committee**
  - **“Denver” vendor NDA visits 8/2009**
  - **SC09 vendor feedback meetings**
  - **Extreme Architecture and Technology Workshop 12/2009**
- **International Exascale Software Project**
  - **Santa Fe, NM 4/2009; Paris, France 6/2009; Tsukuba, Japan 10/2009**







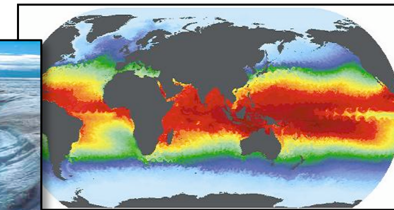
MISSION IMPERATIVES



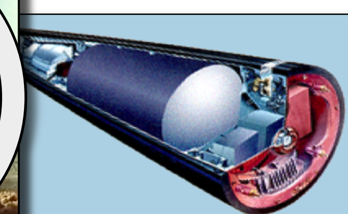
FUNDAMENTAL SCIENCE

DOE mission imperatives require simulation and analysis for policy and decision making

- ***Climate Change***: **Understanding, mitigating and adapting to the effects of global warming**
  - **Sea level rise**
  - **Severe weather**
  - **Regional climate change**
  - **Geologic carbon sequestration**
- ***Energy***: **Reducing U.S. reliance on foreign energy sources and reducing the carbon footprint of energy production**
  - **Reducing time and cost of reactor design and deployment**
  - **Improving the efficiency of combustion energy systems**
- ***National Nuclear Security***: **Maintaining a safe, secure and reliable nuclear stockpile**
  - **Stockpile certification**
  - **Predictive scientific challenges**
  - **Real-time evaluation of urban nuclear detonation**



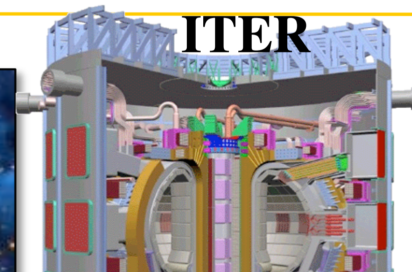


Accomplishing these missions requires exascale resources.

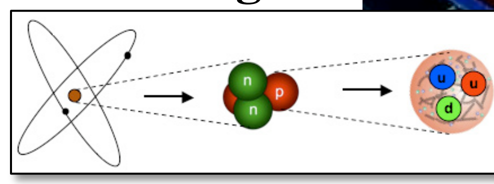
Exascale simulation will enable fundamental advances in basic science.

- High Energy & Nuclear Physics
  - Dark-energy and dark matter
  - Fundamentals of fission fusion reactions
- Facility and experimental design
  - Effective design of accelerators
  - Probes of dark energy and dark matter
  - ITER shot planning and device control
- Materials / Chemistry
  - Predictive multi-scale materials modeling: observation to control
  - Effective, commercial technologies in renewable energy, catalysts, batteries and combustion
- Life Sciences
  - Better biofuels
  - Sequence to structure to function

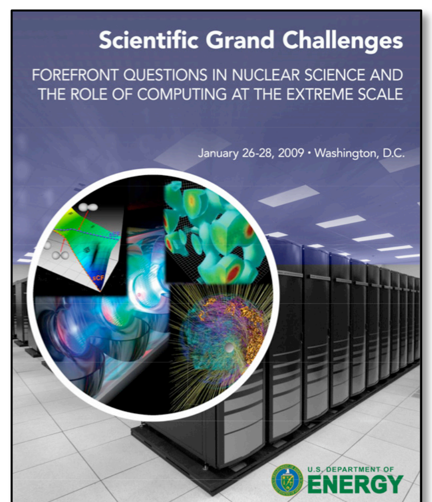
These breakthrough scientific discoveries and facilities require exascale applications and resources.

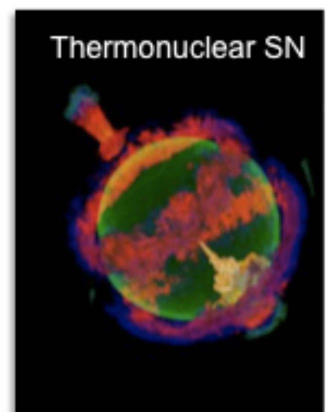


Hubble image of lensing



Structure of nucleons





Potential System Architecture Targets

System attributes	2010	"2015"		"2018"	
System peak	2 Peta	200 Petaflop/sec		1 Exaflop/sec	
Power	6 MW	15 MW		20 MW	
System memory	0.3 PB	5 PB		32-64 PB	
Node performance	125 GF	0.5 TF	7 TF	1 TF	10 TF
Node memory BW	25 GB/s	0.1 TB/sec	1 TB/sec	0.4 TB/sec	4 TB/sec
Node concurrency	12	O(100)	O(1,000)	O(1,000)	O(10,000)
System size (nodes)	18,700	50,000	5,000	1,000,000	100,000
Total Node Interconnect BW	1.5 GB/s	20 GB/sec		200 GB/sec	
MTTI	days	O(1day)		O(1 day)	

Comparison
"2018" vs. Jaguar (2009)

- **500x performance (peak)**
- **100x memory**
- **5000x concurrency**
- **3x power**

All performance increase is based on more parallelism

Keep operating cost about the "same"

Significantly different architecture and software environment

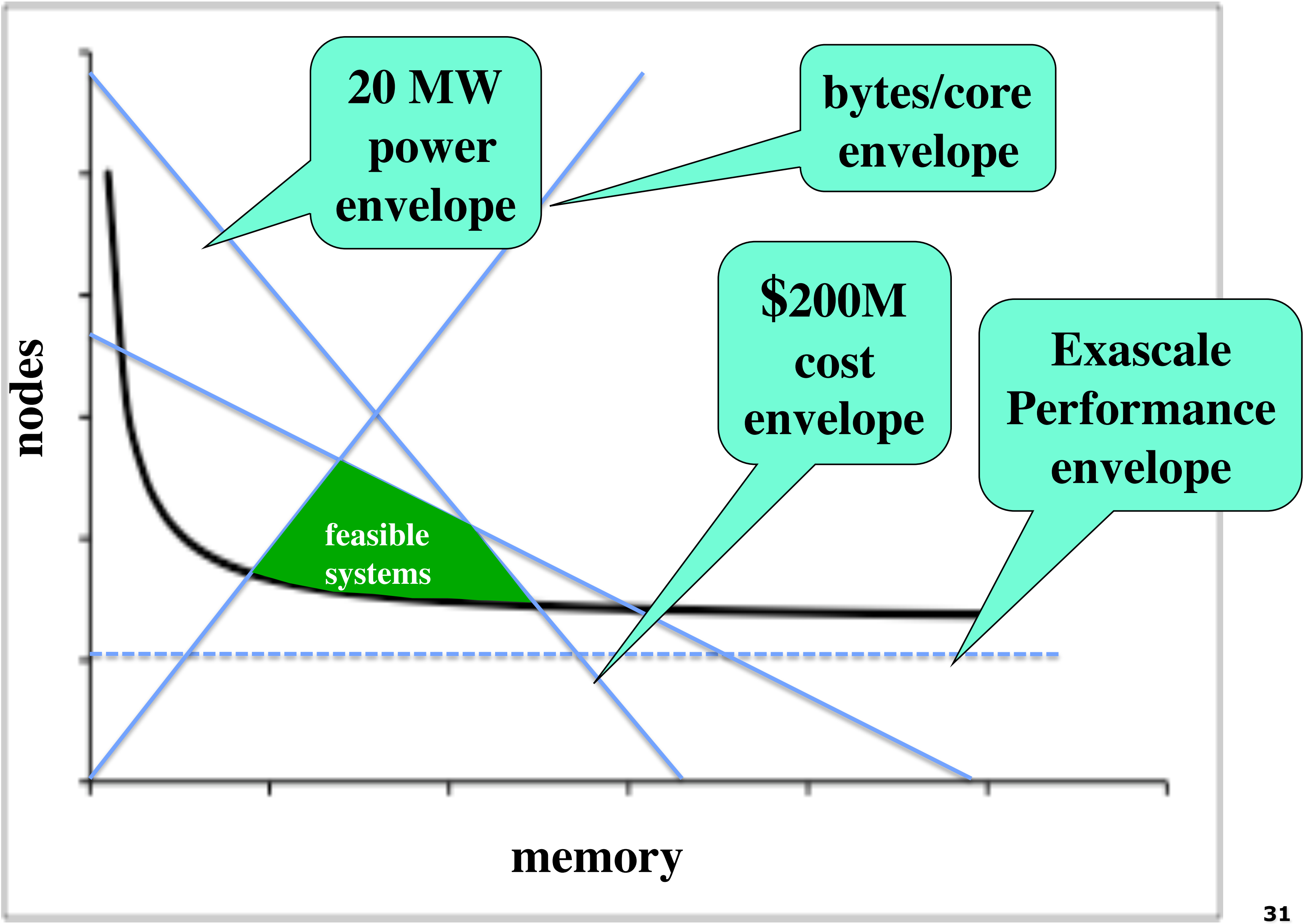
What are critical exascale technology investments?

- **System power** is a first class constraint on exascale system performance and effectiveness.
- M**emory** is an important component of meeting exascale power and applications goals.
- **Programming model**. Early investment in several efforts to decide in 2013 on exascale programming model, allowing exemplar applications effective access to 2015 system for both mission and science.
- **Investment in exascale processor design** to achieve an exascale-like system in 2015.
- **Operating System strategy for exascale** is critical for node performance at scale and for efficient support of new programming models and run time systems.
- **Reliability and resiliency are critical at this** scale and require applications neutral movement of the file system (for check pointing, in particular) closer to the running apps.
- ***HPC co-design strategy and implementation*** *requires a set of a hierarchical performance models and simulators as well as commitment from apps, software and architecture communities.*

Overview

- **From 1999 to 2009: evolution from Teraflops to Petaflops computing**
- **From 2010 to 2020: key technology changes towards Exaflops computing**
- **Impact on Applied Mathematics**
  - **Co-design**

The trade space for exascale is very complex.



Co-design expands the feasible solution space to allow better solutions.

<u>Application driven:</u>
Find the best technology to run this code.
Sub-optimal

Application

- ⬆ **Model**
- ⬆ **Algorithms**
- ⬆ **Code**

Technology

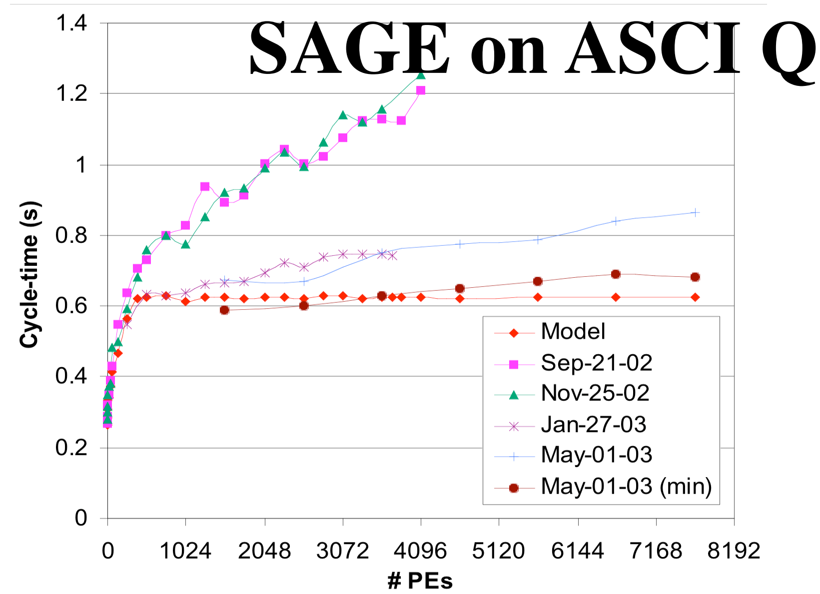
- ⊕ **architecture**
- ⊕ **programming model**
- ⊕ **resilience**
- ⊕ **power**

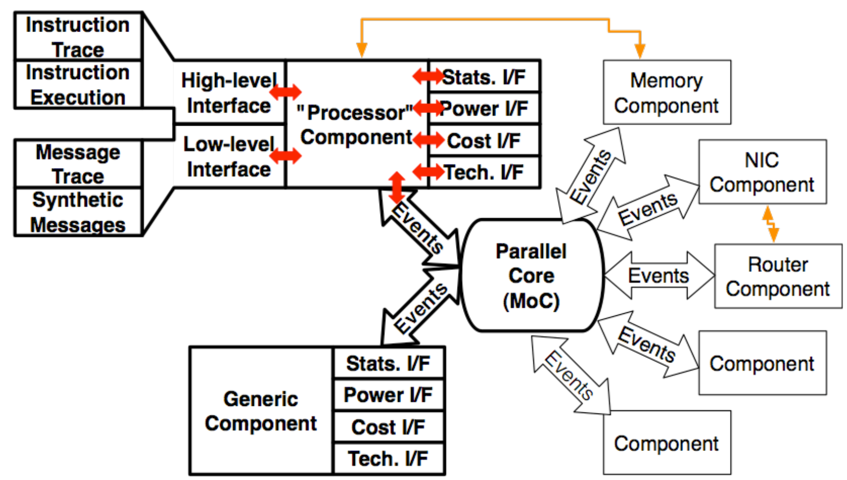
<u>Technology driven:</u>
Fit your application to this technology.
Sub-optimal.

Now, we must expand the co-design space to find better solutions:
•new applications & algorithms,
•better technology and performance.

Hierarchical {application, s/w, h/w} co-simulation a the key for co-design

- **Hierarchical co-simulation capability**
  - Discussions between architecture, software and application groups
  - System level simulation based on analytic models
  - Detailed (e.g. cycle accurate) co-simulation of hardware and applications
- **Opportunity to influence future architectures**
  - Cores/node, threads/core, ALUs/thread
  - Logic layer in stacked memory
  - Interconnect performance
  - Memory/core
  - Processor functionality
- **Current community efforts must work together to provide a complete co-design capability**





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A first step toward co-design was last week's exascale workshop.

- The approach will be to engage experts in computational science, applied mathematics and CS with the goal of
  - Producing a first cut at the characteristics of systems that (a) could be fielded by 2018 and (b) would meet applications' needs
  - Outlining the R&D needed for "co-design" of system architecture, system software and tools, programming frameworks, mathematical models and algorithms, and scientific application codes at the exascale, and
  - Exploring whether this anticipated phase change in technology (like parallel computing in 1990s) provides any opportunities for applications. That is, whether a requirement for revolutionary application design allows new methods, algorithms, and mathematical models to be brought to bear on mission and science questions.

Summary of some priority research directions (PRD)

Black – Crosscutting workshop report

Green – HDS interpretation

- ***Investigate and develop new exascale programming paradigms to support 'billion-way' concurrency***
  - ***Think 10,000 times more parallel***
  - ***Expect MPI+X programming model***
  - ***Think of algorithms that can easily exploit the intra node parallelism, especially if CS researchers develop automatics tools for X***

Summary of some priority research directions (PRD) -- cont.

- ***Re-cast critical applied mathematics algorithms to reflect impact of anticipated macro architecture evolution, such as memory and communication constraints***
  - *Live with less memory/thread and less bandwidth*
- ***Develop new mathematical models and formulations that effectively exploit anticipated exascale hardware architectures***
  - *Add more physics and not just more refinement*
- ***Address numerical analysis questions associated with moving away from bulk-synchronous programs to multi-task approaches***
  - *No more SPMD; think of mapping coarse grain data flow in frameworks*

Summary of some priority research directions (PRD) – cont.

- ***Adapt data analysis algorithms to exascale environments***
- ***Extract essential elements of critical science applications as "mini-applications" that hardware and system software designers can use to understand computational requirements***
- ***Develop tools to simulate emerging architectures for use in co-design***
  - ***Applied mathematicians should be ready to lead co-design teams***

Summary

- **Major Challenges are ahead for extreme computing**
  - **Power**
  - **Parallelism**
  - **… and many others not discussed here**
- **We will need completely new approaches and technologies to reach the Exascale level**
- **This opens up many new opportunities for applied mathematicians**

Shackleton’s Quote on Exascale

Ernest Shackleton’s 1907 ad in London’s Times, recruiting a crew to sail with him on his exploration of the South Pole

“Wanted. Men/women for hazardous architectures. Low wages. Bitter cold. Long hours of software development. Safe return doubtful. Honor and recognition in the event of success.”